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Indispensable monomials of toric ideals and Markov bases

Satoshi Aoki^a, Akimichi Takemura^b, Ruriko Yoshida^c^a *Department of Mathematics and Computer Science, Kagoshima University, Japan*^b *Graduate School of Information Science and Technology, University of Tokyo, Japan*^c *Department of Statistics, University of Kentucky, United States*

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Abstract

Extending the notion of indispensable binomials of a toric ideal [Takemura, Akimichi, Aoki, Satoshi, 2004. Some characterizations of minimal Markov basis for sampling from discrete conditional distributions. *Ann. Inst. Statist. Math.* 56 (1), 1–17; Ohsugi, Hidefumi, Hibi, Takayuki, 2005. Indispensable binomials of finite graphs. *J. Algebra Appl.* 4 (4), 421–434], we define indispensable monomials of a toric ideal and establish some of their properties. They are useful for searching indispensable binomials of a toric ideal and for proving the existence or non-existence of a unique minimal system of binomial generators of a toric ideal. Some examples of indispensable monomials from statistical models for contingency tables are given. © 2007 Elsevier Ltd. All rights reserved.

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1. Introduction

In recent years techniques of computational commutative algebra found applications in many fields, such as optimization (Sturmfels, 1996), computational biology (Pachter and Sturmfels, 2005, 2004; Hoşten et al., 2005), and statistics (Pistone et al., 2001). Particularly, the algebraic view of discrete statistical models has been applied in many statistical problems, including conditional inference (Diaconis and Sturmfels, 1998), disclosure limitation (Sullivant, 2006),

E-mail addresses: aoki@sci.kagoshima-u.ac.jp (S. Aoki), takemura@stat.t.u-tokyo.ac.jp (A. Takemura), ruriko@ms.uky.edu (R. Yoshida).

the maximum likelihood estimation (Hoşten et al., 2005), and parametric inference (Pachter and Sturmfels, 2004). *Algebraic statistics* is a new field, less than a decade old, and its term was coined by Pistone, Riccomagno and Wynn, by the title of their book (Pistone et al., 2001). Computational algebraic statistics has been very actively developed by both algebraists and statisticians since the pioneering work of Diaconis and Sturmfels (1998). For sampling from a finite sample space using Markov-chain Monte Carlo methods, Diaconis and Sturmfels (1998) defined the notion of Markov bases and showed that a Markov basis is equivalent to a system of binomial generators of a toric ideal.

In statistical applications, the number of indeterminates is often large, and at the same time, there exists some inherent symmetry in the toric ideal. For this reason, we encounter computational difficulty in applying Gröbner bases to statistical problems. In particular, even the reduced Gröbner basis of a toric ideal may contain more than several thousands elements, but one might be able to describe the basis concisely using symmetry. For example, Aoki and Takemura (2003) shows that the unique minimal Markov bases for $3 \times 3 \times K$, $K \geq 5$ contingency tables with fixed two-dimensional marginals contain only 6 orbits with respect to the group actions of permuting levels for each axis of contingency tables, while there are 3240, 12085, and 34790 elements in reduced Gröbner bases for $K = 5, 6$, and 7 , respectively. Furthermore in this example the reduced Gröbner basis contains dispensable binomials and is not minimal.

Because of the difficulty mentioned above, the first two authors of this paper have been investigating the question of minimality of Markov bases. In Takemura and Aoki (2004), we defined the notion of indispensable moves, which belong to every Markov basis. We showed that there exists a unique minimal Markov basis if and only if the set of indispensable moves forms a Markov basis. Shortly after, Ohsugi and Hibi investigated indispensable binomials. They showed that the set of indispensable binomials coincides with the intersection of all reduced Gröbner bases with respect to lexicographic term orders in Ohsugi and Hibi (in press). Thus, we are interested in enumerating indispensable binomials of a given toric ideal. However, in general, the enumeration itself is a difficult problem.

This paper proposes the notion of indispensable monomials and investigate some of their properties. The set of indispensable monomials contains all terms of indispensable binomials. Therefore if we could enumerate indispensable monomials, then it would be straightforward to enumerate indispensable binomials. Here it may seem that we are replacing a hard problem by a harder one. Computationally this may well be the case, but we believe that the notion of indispensable monomials may be useful for understanding indispensable binomials and finding the existence of the unique minimal Markov basis.

In Section 2 we will set the notation and summarize relevant results from Takemura and Aoki (2004). In Section 3 we will define indispensable monomials and prove some of their basic properties. Further characterizations of indispensable monomials are given in Section 4 and some nontrivial examples are given in Section 5. We will conclude with some discussions in Section 6.

2. Preliminaries

In this section we will set appropriate notation and then summarize the main results from Takemura and Aoki (2004). Because of the fundamental equivalence mentioned in Diaconis and Sturmfels (1998), we use “system of binomial generators” and “Markov basis” synonymously. Other pairs of synonyms used in this paper are (“binomial”, “move”), (“monomial”, “frequency vector”) and (“indeterminate”, “cell”), as explained below.

2.1. Notation

Because this paper is based on Takemura and Aoki (2004), we follow its notation and terminology in statistical context. Also we adapt some notation in Sturmfels (1996); Miller and Sturmfels (2005). Vectors, through this paper, are column vectors and \mathbf{x}' denotes the transpose of the vector \mathbf{x} .

Let \mathcal{I} be a finite set of $p = |\mathcal{I}|$ elements. Each element of \mathcal{I} is called a *cell*. By ordering cells, we write $\mathcal{I} = \{1, \dots, p\}$ hereafter. A nonnegative integer $x_i \in \mathbb{N} = \{0, 1, \dots\}$ is a *frequency* of a cell i and $\mathbf{x} = (x_1, \dots, x_p)' \in \mathbb{N}^p$ is a *frequency vector* (nonnegative integer vector). We write $|\mathbf{x}| = \sum_{i=1}^p x_i$ to denote the *sample size* of \mathbf{x} . In a framework of similar tests in statistical theory (see Chapter 4 of Lehmann and Romano (2005)), we consider a d -dimensional sufficient statistic defined by

$$\mathbf{t} = \sum_{i=1}^p \mathbf{a}_i x_i,$$

where $\mathbf{a}_i \in \mathbb{Z}^d = \{0, \pm 1, \dots\}^d$ is a d -dimensional fixed integral column vector for $i = 1, \dots, p$. Let $\mathcal{A} = (\mathbf{a}_1, \dots, \mathbf{a}_p) = (a_{ji})$ denote a $d \times p$ integral matrix, where a_{ji} is the j th element of \mathbf{a}_i . Then the *sufficient statistic* \mathbf{t} is written as $\mathbf{t} = \mathcal{A}\mathbf{x}$. The set of frequency vectors for a given sufficient statistic \mathbf{t} is called a *\mathbf{t} -fiber* defined by

$$\mathcal{F}_{\mathbf{t}} = \{\mathbf{x} \in \mathbb{N}^p \mid \mathbf{t} = \mathcal{A}\mathbf{x}\}.$$

A frequency vector $\mathbf{x} (\in \mathbb{N}^p)$ belongs to the fiber $\mathcal{F}_{\mathcal{A}\mathbf{x}}$ by definition. We assume that a toric ideal is homogeneous, i.e. there exists \mathbf{w} such that $\mathbf{w}'\mathbf{a}_i = 1, i = 1, \dots, p$. In this case the sample size of \mathbf{t} is well defined by $|\mathbf{t}| = |\mathbf{x}|$ where $\mathbf{x} \in \mathcal{F}_{\mathbf{t}}$. If the size of $\mathcal{F}_{\mathcal{A}\mathbf{x}}$ is 1, i.e.

$$\mathcal{F}_{\mathcal{A}\mathbf{x}} = \{\mathbf{x}\},$$

we call $\mathbf{x} \in \mathbb{N}^p$ a *1-element fiber*. $|\mathcal{F}_{\mathcal{A}\mathbf{x}}|$ denotes the size (the number of the elements) of the fiber $\mathcal{F}_{\mathcal{A}\mathbf{x}}$. The *support* of \mathbf{x} is denoted by $\text{supp}(\mathbf{x}) = \{i \mid x_i > 0\}$ and the i th coordinate vector is denoted by $\mathbf{e}_i = (0, \dots, 0, 1, 0, \dots, 0)'$, where 1 is in the i th position.

Now, we consider the connection between contingency tables and toric ideals. Let $k[u_1, \dots, u_p] = k[\mathbf{u}]$ denote the polynomial ring in p indeterminates u_1, \dots, u_p over the field k . We identify the indeterminate $u_i \in \mathbf{u}$ with the cell $i \in \mathcal{I}$. For a p -dimensional column vector $\mathbf{x} \in \mathbb{N}^p$ of nonnegative integers, let $\mathbf{u}^{\mathbf{x}} = u_1^{x_1} \cdots u_p^{x_p} \in k[\mathbf{u}]$ denote a monomial. For the sufficient statistic \mathbf{t} , we also treat $\mathbf{t} = (t_1, \dots, t_d)'$ as indeterminates. Let $k[\mathbf{t}^{\pm 1}] = k[t_1, \dots, t_d, t_1^{-1}, \dots, t_d^{-1}]$ denote the Laurent polynomial ring. Then the system of equations $\mathbf{t} = \mathcal{A}\mathbf{x}$ is identified as the mapping $\hat{\pi} : k[\mathbf{u}] \rightarrow k[\mathbf{t}^{\pm 1}]$ defined as $x_i \mapsto \mathbf{t}^{\mathbf{a}_i} = t_1^{a_{1i}} \cdots t_d^{a_{di}}$. The kernel of $\hat{\pi}$ is denoted by $I_{\mathcal{A}} = \ker(\hat{\pi})$ and it is the *toric ideal* associate to the matrix \mathcal{A} .

For statistical applications, it is important to construct a connected Markov chain over the given \mathbf{t} -fiber. Diaconis and Sturmfels (1998) showed that a generator of the toric ideal $I_{\mathcal{A}}$ forms a *Markov basis*, i.e., it gives a connected chain for any \mathbf{t} -fiber.

A p -dimensional integral column vector $\mathbf{z} \in \mathbb{Z}^p$ is a *move* (for \mathcal{A}) if it is in the kernel of \mathcal{A} ,

$$\mathcal{A}\mathbf{z} = \mathbf{0}.$$

Let $\mathbf{z}^+ = (z_1^+, \dots, z_p^+)'$ and $\mathbf{z}^- = (z_1^-, \dots, z_p^-)'$ denote the positive and negative part of a move \mathbf{z} given by

$$z_i^+ = \max(z_i, 0), \quad z_i^- = -\min(z_i, 0),$$

respectively. Then $\mathbf{z} = \mathbf{z}^+ - \mathbf{z}^-$ and \mathbf{z}^+ and \mathbf{z}^- are frequency vectors in the same fiber $\mathcal{F}_{\mathcal{A}\mathbf{z}^+} (= \mathcal{F}_{\mathcal{A}\mathbf{z}^-})$. Adding a move \mathbf{z} to any frequency vector \mathbf{x} does not change its sufficient statistic,

$$\mathcal{A}(\mathbf{x} + \mathbf{z}) = \mathcal{A}\mathbf{x},$$

though $\mathbf{x} + \mathbf{z}$ may not necessarily be a frequency vector. If adding \mathbf{z} to \mathbf{x} does not produce negative elements, we see that $\mathbf{x} \in \mathcal{F}_{\mathcal{A}\mathbf{x}}$ is moved to another element $\mathbf{x} + \mathbf{z} \in \mathcal{F}_{\mathcal{A}\mathbf{x}}$ by \mathbf{z} . In this case, we say that a move \mathbf{z} is *applicable* to \mathbf{x} . \mathbf{z} is applicable to \mathbf{x} if and only if $\mathbf{x} + \mathbf{z} \in \mathcal{F}_{\mathcal{A}\mathbf{x}}$, and equivalently, $\mathbf{x} \geq \mathbf{z}^-$, i.e., $\mathbf{x} - \mathbf{z}^- \in \mathbb{N}^p$. In particular, \mathbf{z} is applicable to \mathbf{z}^- . We say that a move \mathbf{z} *contains* a frequency vector \mathbf{x} if $\mathbf{z}^+ = \mathbf{x}$ or $\mathbf{z}^- = \mathbf{x}$. The sample size of \mathbf{z}^+ (or \mathbf{z}^-) is called a *degree* of \mathbf{z} and denoted by

$$\deg(\mathbf{z}) = |\mathbf{z}^+| = |\mathbf{z}^-|.$$

We also write $|\mathbf{z}| = \sum_{i=1}^p |z_i| = 2 \deg(\mathbf{z})$.

Let $\mathcal{B} = \{\mathbf{z}_1, \dots, \mathbf{z}_L\}$ be a finite set of moves. Let \mathbf{x} and \mathbf{y} be frequency vectors in the same fiber, i.e., $\mathbf{x}, \mathbf{y} \in \mathcal{F}_{\mathcal{A}\mathbf{x}} (= \mathcal{F}_{\mathcal{A}\mathbf{y}})$. Following Takemura and Aoki (2004), we say that \mathbf{y} is *accessible* from \mathbf{x} by \mathcal{B} if there exists a sequence of moves $\mathbf{z}_{i_1}, \dots, \mathbf{z}_{i_k}$ from \mathcal{B} and $\epsilon_j \in \{-1, +1\}$, $j = 1, \dots, k$, satisfying $\mathbf{y} = \mathbf{x} + \sum_{j=1}^k \epsilon_j \mathbf{z}_{i_j}$ and $\mathbf{x} + \sum_{j=1}^h \epsilon_j \mathbf{z}_{i_j} \in \mathcal{F}_{\mathcal{A}\mathbf{x}}$, $h = 1, \dots, k-1$. The latter relation means that the move \mathbf{z}_{i_h} is applicable to $\mathbf{x} + \sum_{j=1}^{h-1} \epsilon_j \mathbf{z}_{i_j}$ for $h = 1, \dots, k$. We write $\mathbf{x} \sim \mathbf{y} \pmod{\mathcal{B}}$ if \mathbf{y} is accessible from \mathbf{x} by \mathcal{B} . An accessibility by \mathcal{B} is an equivalence relation in $\mathcal{F}_{\mathbf{t}}$ for any \mathbf{t} and each $\mathcal{F}_{\mathbf{t}}$ is partitioned into disjoint equivalence classes by \mathcal{B} (see Takemura and Aoki (2004) for details). We call these equivalence classes *\mathcal{B} -equivalence classes* of $\mathcal{F}_{\mathbf{t}}$. Because of symmetry, we also say that \mathbf{x} and \mathbf{y} are *mutually accessible* by \mathcal{B} if $\mathbf{x} \sim \mathbf{y} \pmod{\mathcal{B}}$. Conversely, if \mathbf{x} and \mathbf{y} are not mutually accessible by \mathcal{B} , i.e., \mathbf{x} and \mathbf{y} are elements from two different \mathcal{B} -equivalence classes of $\mathcal{F}_{\mathcal{A}\mathbf{x}}$, we say that a move $\mathbf{z} = \mathbf{x} - \mathbf{y}$ *connects* these two equivalence classes.

A Markov basis is defined by Diaconis and Sturmfels (1998) as follows. A set of finite moves $\mathcal{B} = \{\mathbf{z}_1, \dots, \mathbf{z}_L\}$ is a *Markov basis* if $\mathcal{F}_{\mathbf{t}}$ itself forms one \mathcal{B} -equivalence class for all \mathbf{t} . In other words, if \mathcal{B} is a Markov basis, every $\mathbf{x}, \mathbf{y} \in \mathcal{F}_{\mathbf{t}}$ are mutually accessible by \mathcal{B} for every \mathbf{t} . In statistical applications, a Markov basis makes it possible to construct a connected Markov chain over $\mathcal{F}_{\mathcal{A}\mathbf{x}}$ for any observed frequency data \mathbf{x} .

Diaconis and Sturmfels (1998) showed the existence of a finite Markov basis for any \mathcal{A} and gave an algorithm to compute one. These results were obtained by showing the fact that $\mathcal{B} = \{\mathbf{z}_1, \dots, \mathbf{z}_L\}$ is a Markov basis if and only if the set of binomials $\{\mathbf{u}^{\mathbf{z}_k^+} - \mathbf{u}^{\mathbf{z}_k^-}, k = 1, \dots, L\}$ is a generator of the toric ideal $I_{\mathcal{A}}$ associate to \mathcal{A} . The algorithm in Diaconis and Sturmfels (1998) is based on the elimination theory of polynomial ideals and computation of a Gröbner basis.

2.2. Summary of relevant facts on indispensable moves and minimal Markov bases

In Aoki and Takemura (2003) and Takemura and Aoki (2004, 2005), we have investigated the question on the minimality and unique minimality of Markov bases without computing a Gröbner basis of $I_{\mathcal{A}}$. A Markov basis \mathcal{B} is *minimal* if no proper subset of \mathcal{B} is a Markov basis. A minimal Markov basis always exists, because from any Markov basis, we can remove redundant elements one-by-one until none of the remaining elements can be removed. In defining the minimality of Markov basis, we have to be careful on signs of moves, because minimal \mathcal{B} can contain only one of \mathbf{z} or $-\mathbf{z}$. Also a minimal Markov basis is unique if all minimal Markov bases coincide except for signs of their elements (Takemura and Aoki, 2004).

The structure of the unique minimal Markov basis is given in Takemura and Aoki (2004). Here we will summarize the main results of the paper without proofs. Two particular sets of moves are important. One is the set of moves \mathbf{z} with the same value of the sufficient statistic $\mathbf{t} = \mathcal{A}\mathbf{z}^+ = \mathcal{A}\mathbf{z}^-$, namely

$$\mathcal{B}_{\mathbf{t}} = \{\mathbf{z} \mid \mathcal{A}\mathbf{z}^+ = \mathcal{A}\mathbf{z}^- = \mathbf{t}\},$$

and the other is the set of moves with degree less than or equal to n , namely

$$\mathcal{B}_n = \{\mathbf{z} \mid \deg(\mathbf{z}) \leq n\}.$$

Consider the $\mathcal{B}_{|\mathbf{t}|-1}$ -equivalence classes of $\mathcal{F}_{\mathbf{t}}$ for each \mathbf{t} . We write this equivalence classes of $\mathcal{F}_{\mathbf{t}}$ as $\mathcal{F}_{\mathbf{t}} = \mathcal{F}_{\mathbf{t},1} \cup \dots \cup \mathcal{F}_{\mathbf{t},K_{\mathbf{t}}}$.

Theorem 2.1 (Theorem 2.1 in Takemura and Aoki (2004)). *Let \mathcal{B} be a minimal Markov basis. Then for each \mathbf{t} , $\mathcal{B} \cap \mathcal{B}_{\mathbf{t}}$ consists of $K_{\mathbf{t}} - 1$ moves connecting different $\mathcal{B}_{|\mathbf{t}|-1}$ -equivalence classes of $\mathcal{F}_{\mathbf{t}}$, such that the equivalence classes are connected into a tree by these moves.*

Conversely, choose any $K_{\mathbf{t}} - 1$ moves $\mathbf{z}_{\mathbf{t},1}, \dots, \mathbf{z}_{\mathbf{t},K_{\mathbf{t}}-1}$ connecting different $\mathcal{B}_{|\mathbf{t}|-1}$ -equivalence classes of $\mathcal{F}_{\mathbf{t}}$ such that the equivalence classes are connected into a tree by these moves. Then

$$\bigcup_{\mathbf{t}: K_{\mathbf{t}} \geq 2} \{\mathbf{z}_{\mathbf{t},1}, \dots, \mathbf{z}_{\mathbf{t},K_{\mathbf{t}}-1}\}$$

is a minimal Markov basis.

As pointed out by a referee, this theorem is a consequence of the characterization of minimal generator fibers for toric ideals by Campillo and Pison (1993). From Theorem 2.1, we immediately have a necessary and sufficient condition for the existence of a unique minimal Markov basis.

Corollary 2.1 (Corollary 2.1 in Takemura and Aoki (2004)). *A minimal Markov basis is unique if and only if for each \mathbf{t} , $\mathcal{F}_{\mathbf{t}}$ itself forms one $\mathcal{B}_{|\mathbf{t}|-1}$ -equivalence class or $\mathcal{F}_{\mathbf{t}}$ is a two-element fiber.*

This condition is explicitly expressed by *indispensable moves*.

Definition 2.1. A move $\mathbf{z} = \mathbf{z}^+ - \mathbf{z}^-$ is called indispensable if \mathbf{z}^+ and \mathbf{z}^- form a two-element fiber, i.e., the fiber $\mathcal{F}_{\mathcal{A}\mathbf{z}^+} (= \mathcal{F}_{\mathcal{A}\mathbf{z}^-})$ is written as $\mathcal{F}_{\mathcal{A}\mathbf{z}^+} = \{\mathbf{z}^+, \mathbf{z}^-\}$.

From the above definition and the structure of a minimal Markov basis, one can show that every indispensable move belongs to each Markov basis (Lemma 2.3 in Takemura and Aoki (2004)). Furthermore, by the correspondence between moves and binomials, we define an *indispensable binomial*.

Definition 2.2. A binomial $\mathbf{u}^{\mathbf{z}} = \mathbf{u}^{\mathbf{z}^+} - \mathbf{u}^{\mathbf{z}^-}$ is indispensable if every system of binomial generators of $I_{\mathcal{A}}$ contains $\mathbf{u}^{\mathbf{z}}$ or $-\mathbf{u}^{\mathbf{z}}$.

Clearly, a binomial $\mathbf{u}^{\mathbf{z}}$ is indispensable if and only if a move \mathbf{z} is indispensable. By definition, a set of indispensable moves plays an important role to determine the uniqueness of a minimal Markov basis:

Lemma 2.1 (Corollary 2.2 in Takemura and Aoki (2004)). *The unique minimal Markov basis exists if and only if the set of indispensable moves forms a Markov basis. In this case, the set of indispensable moves is the unique minimal Markov basis.*

Ohsugi and Hibi further investigated indispensable moves (Ohsugi and Hibi, in press, 2005).

Theorem 2.2 (Theorem 2.4 in Ohsugi and Hibi (in press)). *A binomial $\mathbf{u}^{\mathbf{z}}$ is indispensable if and only if either $\mathbf{u}^{\mathbf{z}}$ or $-\mathbf{u}^{\mathbf{z}}$ belongs to the reduced Gröbner basis of $I_{\mathcal{A}}$ for any lexicographic term order on $k[\mathbf{u}]$.*

One can find more details in Ohsugi and Hibi (2005).

3. Definition and some basic properties of indispensable monomials

In this section we will define indispensable monomials. Then we will show two other equivalent conditions for a monomial to be indispensable. We will also prove a result analogous to Theorem 2.4 in Ohsugi and Hibi (in press), that the set of indispensable monomials is characterized as the intersection of monomials in reduced Gröbner bases with respect to all lexicographic term orders. Hereafter, we say that a Markov basis \mathcal{B} contains \mathbf{x} if it contains a move \mathbf{z} containing \mathbf{x} by abusing the terminology.

Firstly we will define an *indispensable monomial*.

Definition 3.1. A monomial $\mathbf{u}^{\mathbf{x}}$ is *indispensable* if every system of binomial generators of $I_{\mathcal{A}}$ contains a binomial f such that $\mathbf{u}^{\mathbf{x}}$ is a term of f .

From this definition, any Markov basis contains all indispensable monomials. Therefore the set of indispensable monomials is finite. Note that both terms of an indispensable binomial $\mathbf{u}^{\mathbf{z}^+} - \mathbf{u}^{\mathbf{z}^-}$ are indispensable monomials, but the converse does not hold in general.

Now we will present an alternative definition.

Definition 3.2. \mathbf{x} is a minimal multi-element if $|\mathcal{F}_{\mathcal{A}\mathbf{x}}| \geq 2$ and $|\mathcal{F}_{\mathcal{A}(\mathbf{x}-\mathbf{e}_i)}| = 1$ for every $i \in \text{supp}(\mathbf{x})$.

Theorem 3.1. \mathbf{x} is an indispensable monomial if and only if \mathbf{x} is a minimal multi-element.

Proof. First, we suppose that \mathbf{x} is a minimal multi-element and want to show that it is an indispensable monomial. Let $n = |\mathbf{x}|$ and consider the fiber $\mathcal{F}_{\mathcal{A}\mathbf{x}}$. We claim that $\{\mathbf{x}\}$ forms a single \mathcal{B}_{n-1} -equivalence class. In order to show this, we argue by contradiction. If $\{\mathbf{x}\}$ does not form a single \mathcal{B}_{n-1} -equivalence class, then there exists a move \mathbf{z} with degree less than or equal to $n - 1$, such that

$$\mathbf{x} + \mathbf{z} = (\mathbf{x} - \mathbf{z}^-) + \mathbf{z}^+ \in \mathcal{F}_{\mathcal{A}\mathbf{x}}.$$

Since $|\mathbf{x}| = n$, $|\mathbf{z}^-| \leq n - 1$, we have $\mathbf{0} \neq \mathbf{x} - \mathbf{z}^-$ and

$$\text{supp}(\mathbf{x}) \cap \text{supp}(\mathbf{x} + \mathbf{z}) \neq \emptyset.$$

Therefore we can choose $i \in \text{supp}(\mathbf{x}) \cap \text{supp}(\mathbf{x} + \mathbf{z})$ such that

$$\mathcal{A}(\mathbf{x} - \mathbf{e}_i) = \mathcal{A}(\mathbf{x} + \mathbf{z} - \mathbf{e}_i), \quad \mathbf{x} - \mathbf{e}_i \neq \mathbf{x} + \mathbf{z} - \mathbf{e}_i.$$

This shows that $|\mathcal{F}_{\mathcal{A}(\mathbf{x}-\mathbf{e}_i)}| \geq 2$, which contradicts the assumption that \mathbf{x} is a minimal multi-element. Therefore we have shown that $\{\mathbf{x}\}$ forms a single \mathcal{B}_{n-1} -equivalence class. Since we are assuming that $|\mathcal{F}_{\mathcal{A}\mathbf{x}}| \geq 2$, there exists some other \mathcal{B}_{n-1} -class in $\mathcal{F}_{\mathcal{A}\mathbf{x}}$. By Theorem 2.1, each Markov basis has to contain a move connecting a one-element equivalence class $\{\mathbf{x}\}$ to other equivalence classes of $\mathcal{F}_{\mathcal{A}\mathbf{x}}$, which implies that each Markov basis has to contain a move \mathbf{z}

containing \mathbf{x} . We now have shown that each minimal multi-element has to be contained in each Markov basis, i.e., a minimal multi-element is an indispensable monomial.

Now we will show the converse. It suffices to show that if \mathbf{x} is not a minimal multi-element, then \mathbf{x} is a dispensable monomial. Suppose that \mathbf{x} is not a minimal multi-element. If \mathbf{x} is a 1-element ($|\mathcal{F}_{\mathcal{A}\mathbf{x}}| = 1$), obviously it is dispensable. Hence assume that $|\mathcal{F}_{\mathcal{A}\mathbf{x}}| \geq 2$. In the case that $\mathcal{F}_{\mathcal{A}\mathbf{x}}$ is a single \mathcal{B}_{n-1} -equivalence class, no move containing \mathbf{x} is needed in a minimal Markov basis by [Theorem 2.1](#). Therefore we only need to consider the case that $\mathcal{F}_{\mathcal{A}\mathbf{x}}$ contains more than one \mathcal{B}_{n-1} -equivalence classes. Because \mathbf{x} is not a minimal multi-element, there exists some $i \in \text{supp}(\mathbf{x})$ such that $|\mathcal{F}_{\mathcal{A}(\mathbf{x}-\mathbf{e}_i)}| \geq 2$. Then there exists $\mathbf{y} \neq \mathbf{x} - \mathbf{e}_i$, such that $\mathcal{A}\mathbf{y} = \mathcal{A}(\mathbf{x} - \mathbf{e}_i)$. Noting that $|\mathbf{y}| = |\mathbf{x} - \mathbf{e}_i| = n - 1$, a move of the form

$$\mathbf{z} = \mathbf{y} - (\mathbf{x} - \mathbf{e}_i) = (\mathbf{y} + \mathbf{e}_i) - \mathbf{x}$$

satisfies $0 < \deg(\mathbf{z}) \leq n - 1$. Then

$$\mathbf{y} + \mathbf{e}_i = \mathbf{x} + \mathbf{z}$$

and \mathbf{x} and $\mathbf{y} + \mathbf{e}_i$ belong to the same \mathcal{B}_{n-1} -equivalence class of $\mathcal{F}_{\mathcal{A}\mathbf{x}}$. Since $\mathbf{x} \neq \mathbf{y} + \mathbf{e}_i$, [Theorem 2.1](#) states that we can construct a minimal Markov basis containing $\mathbf{y} + \mathbf{e}_i$, but not containing \mathbf{x} . Therefore \mathbf{x} is a dispensable monomial. \square

Definition 3.3. \mathbf{x} is a minimal i -lacking 1-element if $|\mathcal{F}_{\mathcal{A}\mathbf{x}}| = 1$, $|\mathcal{F}_{\mathcal{A}(\mathbf{x}+\mathbf{e}_i)}| \geq 2$ and $|\mathcal{F}_{\mathcal{A}(\mathbf{x}+\mathbf{e}_i-\mathbf{e}_j)}| = 1$ for each $j \in \text{supp}(\mathbf{x})$.

We then have the following result.

Theorem 3.2. *The following three conditions are equivalent (1) \mathbf{x} is an indispensable monomial, (2) for each $i \in \text{supp}(\mathbf{x})$, $\mathbf{x} - \mathbf{e}_i$ is a minimal i -lacking 1-element, (3) for some $i \in \text{supp}(\mathbf{x})$, $\mathbf{x} - \mathbf{e}_i$ is a minimal i -lacking 1-element.*

By the previous theorem we can replace the condition (1) by the condition that \mathbf{x} is a minimal multi-element.

Proof. (1) \Rightarrow (2). Suppose that \mathbf{x} is a minimal multi-element. Then for any $i \in \text{supp}(\mathbf{x})$, $\mathbf{x} - \mathbf{e}_i$ is a 1-element and $|\mathcal{F}_{\mathcal{A}((\mathbf{x}-\mathbf{e}_i)+\mathbf{e}_i)}| = |\mathcal{F}_{\mathcal{A}\mathbf{x}}| \geq 2$. If $\mathbf{x} - \mathbf{e}_i$ is not a minimal i -lacking 1-element, then for some $j \in \text{supp}(\mathbf{x} - \mathbf{e}_i)$, $|\mathcal{F}_{\mathcal{A}(\mathbf{x}-\mathbf{e}_j)}| \geq 2$. However $j \in \text{supp}(\mathbf{x} - \mathbf{e}_i) \subset \text{supp}(\mathbf{x})$ and $|\mathcal{F}_{\mathcal{A}(\mathbf{x}-\mathbf{e}_j)}| \geq 2$ contradicts the assumption that \mathbf{x} is a minimal multi-element. It is obvious that (2) \Rightarrow (3).

Finally we will prove (3) \Rightarrow (1). Suppose that for some $i \in \text{supp}(\mathbf{x})$, $\mathbf{x} - \mathbf{e}_i$ is a minimal i -lacking 1-element. Note that $|\mathcal{F}_{\mathcal{A}\mathbf{x}}| = |\mathcal{F}_{\mathcal{A}((\mathbf{x}-\mathbf{e}_i)+\mathbf{e}_i)}| \geq 2$. Now consider $j \in \text{supp}(\mathbf{x})$. If $j \in \text{supp}(\mathbf{x} - \mathbf{e}_i)$ then $|\mathcal{F}_{\mathcal{A}(\mathbf{x}-\mathbf{e}_j)}| = |\mathcal{F}_{\mathcal{A}((\mathbf{x}-\mathbf{e}_i)+\mathbf{e}_i-\mathbf{e}_j)}| = 1$. On the other hand if $j \notin \text{supp}(\mathbf{x} - \mathbf{e}_i)$, then $j = i$ because $j \in \text{supp}(\mathbf{x})$. In this case $|\mathcal{F}_{\mathcal{A}(\mathbf{x}-\mathbf{e}_i)}| = 1$. This shows that \mathbf{x} is a minimal multi-element. \square

Remark 3.1. The following algorithm was suggested by a referee. If there is an oracle to compute a Gröbner basis for a toric idea via a “degree-by-degree” Gröbner basis/Markov basis algorithm, then we have the following algorithm to compute indispensable monomials:

- (1) Using a “degree-by-degree” Gröbner basis/Markov basis algorithm, find a minimal set of lowest degree generators of degree d_0 , then each monomial in these monomials must be indispensable (by [Theorem 3.1](#)).

- (2) Let M_0 be the monomial ideal generated by these monomials. Look at degree $d_1 = d_0 + 1$, and list all monomials not in M_0 of degree d_1 (for example, “basis” command in Macaulay 2).
- (3) Group these monomials with respect to their fibers. Those monomials which come from fibers with more than one element must be indispensable (again by Theorem 3.1).
- (4) Add these monomials to M_0 to obtain M_1 .
- (5) Repeat until a precomputed highest degree for minimal generators is reached.

Theorem 3.2 suggests the following: Find any 1-element \mathbf{x} . It is often the case that each \mathbf{e}_i , $i = 1, \dots, p$, is a 1-element. Randomly choose $1 \leq i \leq p$ and check whether $\mathbf{x} + \mathbf{e}_i$ remains to be a 1-element. Once $|\mathcal{F}_{\mathbf{x}+\mathbf{e}_i}| \geq 2$, then subtract \mathbf{e}_j 's, $j \neq i$, one by one from \mathbf{x} such that it becomes a minimal i -lacking 1-element. We can apply this procedure to find indispensable monomials of some actual statistical problems.

For the rest of this section we will illustrate this procedure with an example of a $2 \times 2 \times 2$ contingency table. Consider the following problem where $p = 8$, $d = 4$ and \mathcal{A} is given as

$$\mathcal{A} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}.$$

In statistics this is known as the complete independence model of $2 \times 2 \times 2$ contingency tables. To see the direct product structure of \mathcal{I} explicitly, we write indeterminates as

$$\mathbf{u} = (u_{111}, u_{112}, u_{121}, u_{122}, u_{211}, u_{212}, u_{221}, u_{222}).$$

To find indispensable monomials for this problem, we start with the monomial $\mathbf{u}^{\mathbf{x}} = u_{111}$ and consider $\mathbf{x} + \mathbf{e}_i$, $i \in \mathcal{I}$. Then we see that

- $u_{111}^2, u_{111}u_{112}, u_{111}u_{121}, u_{111}u_{211}$ are 1-elements,
- $u_{111}u_{122}, u_{111}u_{212}, u_{111}u_{221}$ are 2-elements and
- $u_{111}u_{222}$ is a 4-element.

From this, we found four indispensable monomials, $u_{111}u_{122}, u_{111}u_{212}, u_{111}u_{221}$ and $u_{111}u_{222}$, since each of $u_{122}, u_{212}, u_{221}, u_{222}$ is a 1-element.

Starting from the other monomials, similarly, we can find the following list of indispensable monomials,

- $u_{111}u_{122}, u_{111}u_{212}, u_{111}u_{221}, u_{112}u_{121}, u_{112}u_{211}, u_{112}u_{222}, u_{121}u_{222}, u_{121}u_{211}, u_{122}u_{221}, u_{122}u_{212}, u_{211}u_{222}, u_{212}u_{221}$, each of which is a 2-element monomial, and
- $u_{111}u_{222}, u_{112}u_{221}, u_{121}u_{212}, u_{122}u_{211}$, each of which is a 4-element monomial.

The next step is to consider the newly produced 1-element monomials, $u_{111}^2, u_{111}u_{112}, u_{111}u_{121}, u_{111}u_{211}$ and so on. For each of these monomials, consider adding \mathbf{e}_i , $i \in \mathcal{I}$ one-by-one, checking whether they are multi-element or not. For example, we see that the monomials such as

$$u_{111}^3, u_{111}^2u_{112}, u_{111}u_{112}^2, \dots$$

are again 1-element monomials (and we have to consider these 1-element monomials in the next step). On the other hand, monomials such as

$$u_{111}^2u_{122}, u_{111}u_{112}u_{122}, u_{111}^2u_{222}, u_{111}u_{112}u_{221}, \dots$$

are multi-element monomials. However, it is seen that they are not minimal multi-element, since

$$u_{111}u_{122}, u_{112}u_{122}, u_{111}u_{222}, u_{112}u_{221}, \dots$$

are not 1-element monomials.

To find all indispensable monomials for this problem, we have to repeat the above procedure for monomials of degree 4, 5, Note that this procedure never stops since there are infinite 1-element monomials, such as

$$u_{111}^n, u_{111}^n u_{112}^m, \dots$$

for arbitrary n, m . This is the same difficulty mentioned in Section 2.2 in Takemura and Aoki (2004). Since indispensable monomials belong to any Markov basis, in particular to the Graver basis, Theorem 4.7 in Sturmfels (1996) gives an upper bound for the degree of indispensable monomials and we can stop at this bound.

Finally we will prove the following theorem, which is analogous to Theorem 2.4 in Ohsugi and Hibi (in press) but much easier to prove, since it focuses on a single monomial (rather than a binomial). We need to reproduce only a part of the proof for Theorem 2.4 in Ohsugi and Hibi (in press).

Theorem 3.3. *A monomial \mathbf{x} is indispensable if for every lexicographic order $<_{\text{lex}}$, the reduced Gröbner basis with respect to $<_{\text{lex}}$ contains \mathbf{x} .*

Proof. It suffices to show that if a monomial \mathbf{x} is dispensable, then there exists a lexicographic term order $<_{\text{lex}}$ such that the reduced Gröbner basis $\mathcal{B}_{<_{\text{lex}}}$ does not contain \mathbf{x} . Note that the positive part and negative part of a move belong to the same fiber. Therefore if \mathbf{x} is a 1-element, then no Markov basis contains \mathbf{x} . In particular no Gröbner basis contains \mathbf{x} . Therefore we only need to consider \mathbf{x} such that $|\mathcal{F}_{\mathcal{A}\mathbf{x}}| \geq 2$.

Since we are assuming that \mathbf{x} is dispensable, there exists a Markov basis \mathcal{B} , which does not contain \mathbf{x} . Then there exists a move $\mathbf{z} = \mathbf{z}^+ - \mathbf{z}^- \in \mathcal{B}$, with \mathbf{z} 's sign changed if necessary, such that \mathbf{z} is applicable to \mathbf{x} , i.e., $\mathbf{x} \geq \mathbf{z}^-$. Since \mathcal{B} does not contain \mathbf{x} , $\mathbf{z}^- \neq \mathbf{x}$ and hence \mathbf{z}^- is strictly smaller than \mathbf{x} . Now choose $<_{\text{lex}}$ such that the initial term of \mathbf{z} is \mathbf{z}^- . Then the reduced Gröbner basis with respect to $<_{\text{lex}}$ does not contain \mathbf{x} . \square

4. Further properties of indispensable monomials

In the previous section we gave some basic characterizations of indispensable monomials. In this section we will show further properties of indispensable moves in terms of minimal Markov bases in Takemura and Aoki (2004) and a *norm-reducing Markov basis* in Takemura and Aoki (2005).

Firstly, we will state the following lemma, which is already implicitly used in the proof of Theorem 3.1.

Lemma 4.1. *A monomial $\mathbf{u}^{\mathbf{x}}$ is indispensable if and only if $\mathcal{F}_{\mathcal{A}\mathbf{x}}$ contains more than one $\mathcal{B}_{|\mathbf{x}|-1}$ -equivalence class and the one-element set $\{\mathbf{x}\}$ forms a $\mathcal{B}_{|\mathbf{x}|-1}$ -equivalence class.*

Proof. Suppose that $\mathcal{F}_{\mathcal{A}\mathbf{x}}$ contains more than one $\mathcal{B}_{|\mathbf{x}|-1}$ -equivalence class and the one-element set $\{\mathbf{x}\}$ forms a $\mathcal{B}_{|\mathbf{x}|-1}$ -equivalence class. Then by Theorem 2.1 in Takemura and Aoki (2004), every Markov basis has to connect \mathbf{x} with some other $\mathcal{B}_{|\mathbf{x}|-1}$ -equivalence class of $\mathcal{F}_{\mathcal{A}\mathbf{x}}$. Therefore \mathbf{x} has to appear as a positive part or a negative part of some move \mathbf{z} of the Markov basis.

Conversely, we show that if $\mathcal{F}_{\mathcal{A}_x}$ contains just one $\mathcal{B}_{|x|-1}$ -equivalence class or the equivalence class containing x contains some other vector y , then x is dispensable. In the former case, $\mathcal{F}_{\mathcal{A}_x}$ is already connected by moves of degree less than or equal to $|x| - 1$ and no minimal Markov basis contains a move having x as the positive or the negative part. On the other hand if $y \neq x$ belongs to the same $\mathcal{B}_{|x|-1}$ -equivalence class, then by Theorem 2.1 in Takemura and Aoki (2004), there exists a minimal Markov basis involving y and not x . Therefore x is dispensable. \square

From Takemura and Aoki (2004) it follows that the moves of all minimal Markov bases belong to a common set of fibers. Also, we defined the minimum fiber Markov bases \mathcal{B}_{MF} in Takemura and Aoki (2005) as

$$\mathcal{B}_{MF} = \{z = z^+ - z^- \mid z^+ \not\sim z^- \pmod{\mathcal{B}_{|z|-1}}\}.$$

Based on Lemma 4.1 now we will prove four propositions concerning the fibers in \mathcal{B}_{MF} . In the following four propositions, an equivalence class of a fiber \mathcal{F}_t means a $\mathcal{B}_{|t|-1}$ -equivalence class of \mathcal{F}_t .

Proposition 4.1. *The following three conditions are equivalent: (1) all equivalence classes of all fibers of \mathcal{B}_{MF} are singletons, (2) there exists a minimal Markov basis, such that all monomials contained in the basis are indispensable. (3) for all minimal Markov bases, all monomials contained in the basis are indispensable.*

Proof. Obviously (3) \Rightarrow (2). (2) \Rightarrow (1) follows from Lemma 4.1 because a minimal basis has to connect all equivalence classes of each fiber of \mathcal{B}_{MF} into a tree. To show that (1) \Rightarrow (3), we again use the fact that a minimal basis has to connect all equivalence classes of each fiber of \mathcal{B}_{MF} into a tree. If all equivalence classes of a fiber are singletons, then both terms of a move connecting two equivalence classes are indispensable. This completes the proof. \square

Proposition 4.2. *There exists a minimal Markov basis such that each move of the basis contains an indispensable monomial if and only if each fiber of \mathcal{B}_{MF} contains a singleton equivalence class.*

Proof. Let \mathcal{B} be a minimal Markov basis such that each move of \mathcal{B} contains an indispensable monomial. This monomial forms a singleton equivalence class. Therefore each fiber of \mathcal{B}_{MF} contains a singleton equivalence class. Conversely if each fiber of \mathcal{B}_{MF} contains a singleton equivalence class, we can construct a tree which connects each equivalence class of the fiber to the singleton equivalence class. Then the resulting minimal Markov basis has the property that each move of the basis contains an indispensable monomial. \square

Proposition 4.3. *Every move of any minimal Markov basis contains an indispensable monomial if and only if all but one equivalence classes of each fiber of \mathcal{B}_{MF} are singletons.*

Proof. If all but one equivalence classes of each fiber of \mathcal{B}_{MF} are singletons, then in connecting these equivalence classes into a tree, each move has to contain an indispensable monomial. On the other hand if there exist two non-singleton equivalence classes in a fiber, then we can construct a minimal Markov basis containing a move connecting these two equivalence classes. This move does not contain an indispensable monomial. \square

Next, we consider indispensable monomials in terms of norm-reduction introduced in Takemura and Aoki (2005). We will give a definition of a norm-reducing Markov basis here (see Takemura and Aoki (2005) for details).

Definition 4.1. A set of moves \mathcal{B} is 1-norm-reducing if for all \mathbf{t} and for all $\mathbf{x}, \mathbf{y} \in \mathcal{F}_{\mathbf{t}}$ with $\mathbf{x} \neq \mathbf{y}$, there exist some $\mathbf{z} \in \mathcal{B}$ and $\epsilon \in \{-1, +1\}$ satisfying either

$$|(\mathbf{x} + \epsilon\mathbf{z}) - \mathbf{y}| < |\mathbf{x} - \mathbf{y}|$$

or

$$|\mathbf{x} - (\mathbf{y} + \epsilon\mathbf{z})| < |\mathbf{x} - \mathbf{y}|.$$

It is easy to show that, if \mathcal{B} is 1-norm-reducing, then it is a Markov basis (see Proposition 1 in Takemura and Aoki (2005)). Therefore we call \mathcal{B} a *1-norm-reducing Markov basis* if it is 1-norm-reducing. An example of 1-norm-reducing Markov basis is the Graver basis (see Proposition 2 in Takemura and Aoki (2005)). Now we will give a characterization of indispensable monomials in terms of the norm-reduction.

Proposition 4.4. A move, whose both monomials are indispensable, belongs to each 1-norm-reducing Markov basis.

Proof. Let $\mathbf{z} = \mathbf{z}^+ - \mathbf{z}^-$ be a move such that both \mathbf{z}^+ and \mathbf{z}^- are indispensable, i.e., $\{\mathbf{z}^+\}$ and $\{\mathbf{z}^-\}$ are singleton equivalence classes of a fiber. If a Markov basis \mathcal{B} does not contain \mathbf{z} , then it cannot decrease the distance between \mathbf{z}^+ and \mathbf{z}^- . Therefore \mathcal{B} is not 1-norm-reducing. \square

Finally, we give a further definition, which is similar to a minimal multi-element.

Definition 4.2. $\mathcal{F}_{\mathbf{t}}$ is a minimal multi-element fiber if $|\mathcal{F}_{\mathbf{t}}| \geq 2$ and $|\mathbf{t}| = 1$ or $|\mathcal{F}_{\mathbf{t}}| \geq 2$, $|\mathcal{F}_{\mathbf{t}_1}| = |\mathcal{F}_{\mathbf{t}_2}| = 1$ for any $\mathbf{t} = \mathbf{t}_1 + \mathbf{t}_2$ satisfying $|\mathcal{F}_{\mathbf{t}_1}|, |\mathcal{F}_{\mathbf{t}_2}| \geq 1$.

The meaning of this definition is as follows. Suppose $|\mathcal{F}_{\mathbf{t}_1}| \geq 2$ and $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{F}_{\mathbf{t}_1}$. Then for any $\mathbf{t}_2 = \mathcal{A}\mathbf{x}_3$, $|\mathcal{F}_{\mathbf{t}_1+\mathbf{t}_2}| \geq 2$ follows since $\mathbf{x}_1 + \mathbf{x}_3, \mathbf{x}_2 + \mathbf{x}_3 \in \mathcal{F}_{\mathbf{t}_1+\mathbf{t}_2}$. Note that the former case, $|\mathcal{F}| \geq 2, |\mathbf{t}| = 1$, corresponds to the case $\mathcal{F}_{\mathbf{t}} \ni \mathbf{e}_i, \mathbf{e}_j, \dots$, for some i, j, \dots . One of the situations that this special case appears is $\mathcal{A} = [1, \dots, 1]$. Hereafter, we only consider the problem that $|\mathbf{t}| \geq 2$ holds for every minimal multi-element fiber $\mathcal{F}_{\mathcal{A}\mathbf{t}}$. In other words, we assume that every \mathbf{e}_i is a one-element. In this case, minimal multi-element fiber is characterized as follows.

Proposition 4.5. $\mathcal{F}_{\mathbf{t}}$ is a minimal multi-element fiber if and only if all the elements in $\mathcal{F}_{\mathbf{t}}$ are indispensable monomials.

Proof. Suppose all the elements in $\mathcal{F}_{\mathbf{t}}$ are indispensable monomials and $\mathbf{t} = \mathbf{t}_1 + \mathbf{t}_2$ where $|\mathcal{F}_{\mathbf{t}_1}| \geq 2, |\mathcal{F}_{\mathbf{t}_2}| \geq 1$. Write $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{F}_{\mathbf{t}_1}$ and $\mathbf{x}_3 \in \mathcal{F}_{\mathbf{t}_2}$. In this case, both $\mathbf{x}_1 + \mathbf{x}_3$ and $\mathbf{x}_2 + \mathbf{x}_3$ are in $\mathcal{F}_{\mathbf{t}}$ and therefore indispensable monomials by the assumption. However, for any $i \in \text{supp}(\mathbf{x}_3)$, $\mathbf{x}_1 + \mathbf{x}_3 - \mathbf{e}_i$ and $\mathbf{x}_2 + \mathbf{x}_3 - \mathbf{e}_i$ are again in the same fiber, which contradicts the assumption that $\mathbf{x}_1 + \mathbf{x}_3$ and $\mathbf{x}_2 + \mathbf{x}_3$ are minimal multi-elements.

Conversely, suppose $\mathcal{F}_{\mathbf{t}}$ is a minimal multi-element fiber and $\mathbf{x} \in \mathcal{F}_{\mathbf{t}}$ is dispensable. In this case, since \mathbf{x} is not a minimal multi-element, there exists some \mathbf{e}_i satisfying $|\mathcal{F}_{\mathcal{A}(\mathbf{x}-\mathbf{e}_i)}| \geq 2$. Therefore we have $\mathcal{A}\mathbf{x} = \mathcal{A}(\mathbf{x} - \mathbf{e}_i) + \mathcal{A}\mathbf{e}_i$, i.e., $\mathbf{t} = \mathbf{t}_1 + \mathbf{t}_2$ where $\mathbf{t}_1 = \mathcal{A}(\mathbf{x} - \mathbf{e}_i)$ and $\mathbf{t}_2 = \mathcal{A}\mathbf{e}_i$, which contradicts the assumption that $\mathcal{F}_{\mathbf{t}}$ is a minimal multi-element fiber. \square

5. Examples

In this section, we will give some indispensable monomials and dispensable monomials in minimal Markov bases for some statistical models. As is stated in Takemura and Aoki

(2004), there are some models where a minimal Markov basis is uniquely determined, and some models where it is not uniquely determined. Furthermore, by considering the indispensability of monomials contained in minimal Markov bases, we can classify Markov bases by the indispensability of monomials as follows.

- Case 1. A minimal Markov basis is uniquely determined, i.e., the set of indispensable moves forms a Markov basis.
- Case 2. A minimal Markov basis is not uniquely determined, but all the monomials in minimal Markov bases are the same and indispensable. In this case, all equivalence classes of each fiber of \mathcal{B}_{MF} are singletons.
- Case 3. A minimal Markov basis is not uniquely determined, and they contain some moves where their positive or negative parts are dispensable monomials. In this case, some equivalence classes of some fiber of \mathcal{B}_{MF} are not singletons.

We will show examples for Case 2 and Case 3 in this section. As for Case 1, the set of the positive and negative parts of indispensable binomials is the set of indispensable monomials. One of the most simple examples for Case 1 is an independence model of two-way contingency tables. A quite difficult example is a no three-factor interaction model of three-way contingency tables, i.e., the case that $\mathcal{A}\mathbf{x}$ is the two-dimensional marginal totals of three-way contingency tables \mathbf{x} . For this example, minimal Markov bases for some small sizes of \mathbf{x} is shown to be unique (see Aoki and Takemura (2003) for the example of $3 \times 3 \times K$ case). Indispensable monomials for Case 1 clearly coincide the positive and negative parts of indispensable binomials.

5.1. Examples of Case 2

One-way contingency tables with fixed totals. First we consider the simplest example given by $\mathcal{A} = 1'_p$, $p > 2$, where $1_p = (1, \dots, 1)'$ is the p -dimensional vector consisting 1's. As is shown in Takemura and Aoki (2004), minimal Markov bases for this problem contain dispensable moves only, which connect p elements,

$$\{u_1, u_2, \dots, u_p\}$$

into a tree. It is also obvious that these p monomials are all indispensable.

Complete independence models of three-way contingency tables. We will show a generalization of the problem considered at the end of Section 3.

Let \mathbf{x} be a frequency vector for $I \times J \times K$ contingency tables and let

$$\mathcal{I} = \{ijk \mid 1 \leq i \leq I, 1 \leq j \leq J, 1 \leq k \leq K\}.$$

\mathcal{A} is given as

$$\mathcal{A} = \begin{bmatrix} 1'_I \otimes 1'_J \otimes E_K \\ 1'_I \otimes E_J \otimes 1'_K \\ E_I \otimes 1'_J \otimes 1'_K \end{bmatrix},$$

where E_n is the $n \times n$ identity matrix. The minimum fiber Markov basis for this problem is given in Takemura and Aoki (2005) as

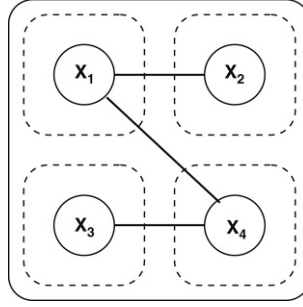


Fig. 1. Illustration of the 4-element fiber $\mathcal{F}_{i_1 i_2 j_1 j_2 k_1 k_2}$ of the complete independence model of three-way contingency tables. The four circles are four monomials, where $\mathbf{x}_1 = u_{i_1 j_1 k_1} u_{i_2 j_2 k_2}$, $\mathbf{x}_2 = u_{i_1 j_1 k_2} u_{i_2 j_2 k_1}$, $\mathbf{x}_3 = u_{i_1 j_2 k_1} u_{i_2 j_1 k_2}$ and $\mathbf{x}_4 = u_{i_1 j_2 k_2} u_{i_2 j_1 k_1}$. Each monomial forms \mathcal{B}_1 -equivalence class of the fiber by itself represented by the dotted square. We will use this convention in all forthcoming figures. The thick lines mean a choice of three dispensable moves, $\{\mathbf{x}_1 - \mathbf{x}_2, \mathbf{x}_1 - \mathbf{x}_4, \mathbf{x}_3 - \mathbf{x}_4\}$, which is an example of choices for constructing a minimal Markov basis.

$$\begin{aligned}
 \mathcal{B}_{\text{MF}} &= \mathcal{B}_{\text{IDP}} \cup \mathcal{B}^*, \\
 \mathcal{B}_{\text{IDP}} &= \{u_{i_1 j_1 k_1} u_{i_2 j_2 k_2} - u_{i_1 j_1 k_2} u_{i_2 j_2 k_1}, j_1 \neq j_2, k_1 \neq k_2\} \\
 &\quad \cup \{u_{i_1 j_1 k_1} u_{i_2 j_2 k_2} - u_{i_1 j_2 k_1} u_{i_2 j_1 k_2}, i_1 \neq i_2, k_1 \neq k_2\} \\
 &\quad \cup \{u_{i_1 j_1 k_1} u_{i_2 j_2 k_2} - u_{i_1 j_2 k_2} u_{i_2 j_1 k_1}, i_1 \neq i_2, j_1 \neq j_2\}, \\
 \mathcal{B}^* &= \{u_{i_1 j_1 k_1} u_{i_2 j_2 k_2} - u_{i_1 j_1 k_2} u_{i_2 j_2 k_1}, u_{i_1 j_1 k_1} u_{i_2 j_2 k_2} - u_{i_1 j_2 k_1} u_{i_2 j_1 k_2}, \\
 &\quad u_{i_1 j_1 k_1} u_{i_2 j_2 k_2} - u_{i_1 j_2 k_2} u_{i_2 j_1 k_1}, u_{i_1 j_1 k_2} u_{i_2 j_2 k_1} - u_{i_1 j_2 k_1} u_{i_2 j_1 k_2}, \\
 &\quad u_{i_1 j_1 k_2} u_{i_2 j_2 k_1} - u_{i_1 j_2 k_2} u_{i_2 j_1 k_1}, u_{i_1 j_2 k_1} u_{i_2 j_1 k_2} - u_{i_1 j_2 k_2} u_{i_2 j_1 k_1}, \\
 &\quad i_1 \neq i_2, j_1 \neq j_2, k_1 \neq k_2\}.
 \end{aligned}$$

Here, \mathcal{B}_{IDP} is the set of indispensable moves. \mathcal{B}^* is the set of all degree 2 moves which connect all elements of the four-elements fiber

$$\begin{aligned}
 \mathcal{F}_{i_1 i_2 j_1 j_2 k_1 k_2} &= \{\mathbf{x} = \{x_{ijk}\} \mid x_{i_1 \cdot \cdot} = x_{i_2 \cdot \cdot} = x_{\cdot j_1 \cdot} = x_{\cdot j_2 \cdot} = x_{\cdot \cdot k_1} = x_{\cdot \cdot k_2} = 1\} \\
 &= \{u_{i_1 j_1 k_1} u_{i_2 j_2 k_2}, u_{i_1 j_1 k_2} u_{i_2 j_2 k_1}, u_{i_1 j_2 k_1} u_{i_2 j_1 k_2}, u_{i_1 j_2 k_2} u_{i_2 j_1 k_1}\}.
 \end{aligned}$$

The minimal Markov basis in this case consists of \mathcal{B}_{IDP} and three moves for each $i_1 \neq i_2, j_1 \neq j_2$, and $k_1 \neq k_2$, which connect four elements of $\mathcal{F}_{i_1 i_2 j_1 j_2 k_1 k_2}$ into a tree. In this case, the four elements of $\mathcal{F}_{i_1 i_2 j_1 j_2 k_1 k_2}$ are different \mathcal{B}_1 -equivalence classes, which are obviously singletons. Therefore the set of indispensable monomials for this problem is

$$\{u_{i_1 j_1 k_1} u_{i_2 j_2 k_2}, u_{i_1 j_1 k_2} u_{i_2 j_2 k_1}, u_{i_1 j_2 k_1} u_{i_2 j_1 k_2}, u_{i_1 j_2 k_2} u_{i_2 j_1 k_1}, i_1 \neq i_2, j_1 \neq j_2, k_1 \neq k_2\}$$

in addition to the positive and negative components of \mathcal{B}_{IDP} . Fig. 1 illustrates the fiber $\mathcal{F}_{i_1 i_2 j_1 j_2 k_1 k_2}$.

Hardy–Weinberg model. Another example considered in Takemura and Aoki (2004) is the Hardy–Weinberg model for I alleles, i.e.,

$$\mathbf{x} = (x_{11}, x_{12}, \dots, x_{1I}, x_{22}, x_{23}, \dots, x_{2I}, x_{33}, \dots, x_{II})'$$

and

$$\mathcal{A} = (\mathcal{A}_I \mathcal{A}_{I-1} \cdots \mathcal{A}_1), \quad \mathcal{A}_k = (O_{k \times (I-k)} B_k')',$$

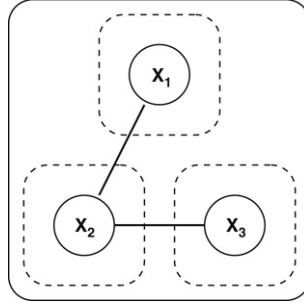


Fig. 2. Illustration of the 3-element fiber $\mathcal{F}_{i_1 i_2 i_3 i_4}$ of the Hardy–Weinberg models. The three circles are three monomials, $\mathbf{x}_1 = u_{i_1 i_2} u_{i_3 i_4}$, $\mathbf{x}_2 = u_{i_1 i_3} u_{i_2 i_4}$ and $\mathbf{x}_3 = u_{i_1 i_4} u_{i_2 i_3}$. The thick lines are the two dispensable moves, $\{\mathbf{x}_1 - \mathbf{x}_2, \mathbf{x}_2 - \mathbf{x}_3\}$.

where B_k is the following $k \times k$ square matrix

$$B_k = \begin{bmatrix} 2 & 1 & 1 & \cdots & 1 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix}.$$

As is stated in Takemura and Aoki (2004), a minimal Markov basis for this case is not unique, and the minimum fiber Markov basis is:

$$\begin{aligned} \mathcal{B}_{\text{MF}} &= \mathcal{B}_{\text{IDP}} \cup \mathcal{B}^*, \\ \mathcal{B}_{\text{IDP}} &= \{u_{i_1 i_1} u_{i_2 i_3} - u_{i_1 i_2} u_{i_1 i_3}, u_{i_1 i_1} u_{i_2 i_2} - u_{i_1 i_2}^2\}, \\ \mathcal{B}^* &= \{u_{i_1 i_2} u_{i_3 i_4} - u_{i_1 i_3} u_{i_2 i_4}, u_{i_1 i_2} u_{i_3 i_4} - u_{i_1 i_4} u_{i_2 i_3}, u_{i_1 i_3} u_{i_2 i_4} - u_{i_1 i_4} u_{i_2 i_3}\}, \end{aligned}$$

where i_1, i_2, i_3, i_4 are all distinct, and $u_{ij} = u_{ji}$ for $i > j$. Here, \mathcal{B}^* is the set of all degree 2 moves which connect all of the elements of the three-element fiber

$$\mathcal{F}_{i_1 i_2 i_3 i_4} = \{u_{i_1 i_2} u_{i_3 i_4}, u_{i_1 i_3} u_{i_2 i_4}, u_{i_1 i_4} u_{i_2 i_3}\}.$$

Again, these three elements of $\mathcal{F}_{i_1 i_2 i_3 i_4}$ form singleton \mathcal{B}_1 -equivalence classes of it by themselves, and are indispensable monomials. Fig. 2 illustrates the fiber $\mathcal{F}_{i_1 i_2 i_3 i_4}$.

5.2. Examples of Case 3

Some examples for this case are found in the hierarchical models of $2 \times 2 \times 2 \times 2$ contingency tables considered in Aoki and Takemura (in press). First we will show one of them as an example of Case 3. By modifying the example, we will show another example of the situation considered in Proposition 4.3, i.e., the situation that some dispensable moves contain both indispensable and dispensable monomials as their positive and negative parts.

12/13/23/34 model of $2 \times 2 \times 2 \times 2$ contingency tables. Let \mathbf{x} be a frequency vector for $2 \times 2 \times 2 \times 2$ contingency tables ($p = 16$). We write the indeterminates with respect to a lexicographic order as

$$\mathbf{u} = \{u_{1111}, u_{1112}, u_{1121}, u_{1122}, u_{1211}, \dots, u_{2222}\}.$$

Consider the model of $d = 9$ given as

$$\mathcal{A} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}.$$

For this case, there are 12 indispensable moves of degree 2 and 4 indispensable moves of degree 4, but the set of indispensable moves does not form a Markov basis. In addition to the indispensable moves, we have to consider moves connecting 4-element fiber

$$\mathcal{F}^1 = \{u_{1111}u_{1221}u_{2121}u_{2212}, u_{1112}u_{1221}u_{2121}u_{2211}, u_{1121}u_{1211}u_{2112}u_{2221}, u_{1121}u_{1212}u_{2111}u_{2221}\}$$

and 8-element fiber

$$\mathcal{F}^2 = \{u_{1111}u_{1221}u_{2122}u_{2212}, u_{1112}u_{1222}u_{2121}u_{2211}, u_{1111}u_{1222}u_{2121}u_{2212}, u_{1112}u_{1221}u_{2122}u_{2211}, u_{1121}u_{1211}u_{2112}u_{2222}, u_{1122}u_{1212}u_{2111}u_{2221}, u_{1121}u_{1212}u_{2111}u_{2222}, u_{1122}u_{1211}u_{2112}u_{2221}\}.$$

For \mathcal{F}^1 , we have \mathcal{B}_3 -equivalence classes of it as

$$\mathcal{F}^1 = \{u_{1111}u_{1221}u_{2121}u_{2212}, u_{1112}u_{1221}u_{2121}u_{2211}\} \cup \{u_{1121}u_{1211}u_{2112}u_{2221}, u_{1121}u_{1212}u_{2111}u_{2221}\}.$$

Therefore these 4 elements are dispensable monomials. In fact, we can find an element of minimal Markov basis not containing $u_{1111}u_{1221}u_{2121}u_{2212}$, for example, as

$$u_{1112}u_{1221}u_{2121}u_{2211} - u_{1121}u_{1211}u_{2112}u_{2221}.$$

Similarly for \mathcal{F}^2 , \mathcal{B}_3 -equivalence classes of it are given as

$$\mathcal{F}^2 = \{u_{1111}u_{1221}u_{2122}u_{2212}, u_{1112}u_{1222}u_{2121}u_{2211}, u_{1111}u_{1222}u_{2121}u_{2212}, u_{1112}u_{1221}u_{2122}u_{2211}\} \cup \{u_{1121}u_{1211}u_{2112}u_{2222}, u_{1122}u_{1212}u_{2111}u_{2221}, u_{1121}u_{1212}u_{2111}u_{2222}, u_{1122}u_{1211}u_{2112}u_{2221}\}.$$

Figs. 3 and 4 illustrate the fiber \mathcal{F}^1 and \mathcal{F}^2 , respectively.

12/13/23/34 model of $2 \times 2 \times 2 \times 2$ contingency tables with a structural zero cell. We modify the previous example by introducing a structural zero cell, $x_{111} \equiv 0$. This situation corresponds to removing the indeterminate u_{1111} and the first column of \mathcal{A} as

$$\mathbf{u} = \{u_{1112}, u_{1121}, u_{1122}, u_{1211}, \dots, u_{2222}\},$$

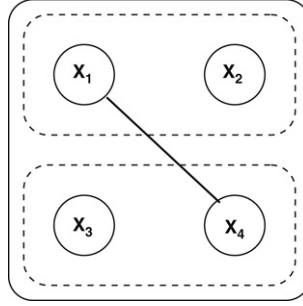


Fig. 3. Illustration of the 4-element fiber \mathcal{F}^1 of 12/13/23/34 model of $2 \times 2 \times 2 \times 2$ contingency tables. The four monomials are $\mathbf{x}_1 = u_{1111}u_{1221}u_{2121}u_{2212}$, $\mathbf{x}_2 = u_{1112}u_{1221}u_{2121}u_{2211}$, $\mathbf{x}_3 = u_{1121}u_{1211}u_{2112}u_{2221}$ and $\mathbf{x}_4 = u_{1121}u_{1212}u_{2111}u_{2221}$. $\{\mathbf{x}_1, \mathbf{x}_2\}$ and $\{\mathbf{x}_3, \mathbf{x}_4\}$ form \mathcal{B}_3 -equivalence classes of the fiber. The thick line is a dispensable move, $\mathbf{x}_1 - \mathbf{x}_4$.

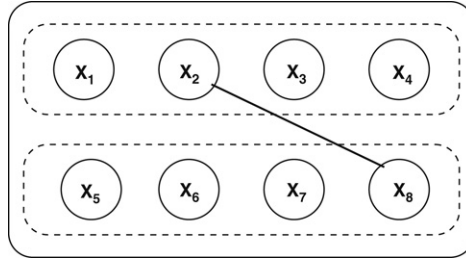


Fig. 4. Illustration of the 8-element fiber \mathcal{F}^2 of 12/13/23/34 model of $2 \times 2 \times 2 \times 2$ contingency tables. The eight monomials are $\mathbf{x}_1 = u_{1111}u_{1221}u_{2122}u_{2212}$, $\mathbf{x}_2 = u_{1112}u_{1222}u_{2121}u_{2211}$, $\mathbf{x}_3 = u_{1111}u_{1222}u_{2121}u_{2212}$, $\mathbf{x}_4 = u_{1112}u_{1221}u_{2122}u_{2211}$, $\mathbf{x}_5 = u_{1121}u_{1211}u_{2112}u_{2222}$, $\mathbf{x}_6 = u_{1122}u_{1212}u_{2111}u_{2221}$, $\mathbf{x}_7 = u_{1121}u_{1212}u_{2111}u_{2222}$ and $\mathbf{x}_8 = u_{1122}u_{1211}u_{2112}u_{2221}$. $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$ and $\{\mathbf{x}_5, \mathbf{x}_6, \mathbf{x}_7, \mathbf{x}_8\}$ form \mathcal{B}_3 -equivalence classes of the fiber. The thick line is a dispensable move, $\mathbf{x}_2 - \mathbf{x}_8$.

$$A = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}.$$

In this case, the fiber \mathcal{F}^1 in the previous example is modified to a 3-element fiber,

$$\mathcal{F}^{1*} = \{u_{1112}u_{1221}u_{2121}u_{2211}, u_{1121}u_{1211}u_{2112}u_{2221}, u_{1121}u_{1212}u_{2111}u_{2221}\}.$$

Since \mathcal{F}^{1*} still has different \mathcal{B}_3 -equivalence classes, we have to consider moves connecting the elements of \mathcal{F}^{1*} to construct a minimal Markov basis. In this case, \mathcal{B}_3 -equivalence classes of \mathcal{F}^{1*} are given as

$$\mathcal{F}^{1*} = \{u_{1112}u_{1221}u_{2121}u_{2211}\} \cup \{u_{1121}u_{1211}u_{2112}u_{2221}, u_{1121}u_{1212}u_{2111}u_{2221}\}.$$

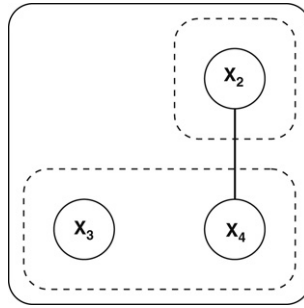


Fig. 5. Illustration of the 3-element fiber \mathcal{F}^{1*} of 12/13/23/34 model of $2 \times 2 \times 2 \times 2$ contingency tables with structural zero cell. This fiber is constructed by removing element x_1 from \mathcal{F}^1 . In this case, $\{x_2\}$ and $\{x_3, x_4\}$ form \mathcal{B}_3 -equivalence classes of the fiber. The thick line means a choice of a dispensable move, $x_2 - x_4$. Another possibility of constructing a minimal Markov basis is to choose a dispensable move, $x_2 - x_3$. The monomial x_2 is included in any minimal Markov basis, and is an indispensable monomial.

Therefore a minimal Markov basis for this problem has to contain either

$$u_{1112}u_{1221}u_{2121}u_{2211} - u_{1121}u_{1211}u_{2112}u_{2221}$$

or

$$u_{1112}u_{1221}u_{2121}u_{2211} - u_{1121}u_{1212}u_{2111}u_{2221}.$$

The above two moves are dispensable, and the negative parts of both moves are also dispensable monomials, whereas the positive part, $u_{1112}u_{1221}u_{2121}u_{2211}$, is an indispensable monomial. Fig. 5 illustrates the fiber \mathcal{F}^{1*} .

6. Some discussions

In this paper, the concept of indispensable monomials is introduced, by extending the notion of indispensable binomials. Both in the framework of Markov bases and toric ideals, the indispensable monomial plays an important role since it has to be included in all Markov bases or generators of toric ideals. It is true that enumerating indispensable monomials is as difficult as enumerating indispensable binomials.

Note that, by the notion of indispensable monomials, we can characterize a dispensable binomial as (i) a difference of two dispensable monomials, (ii) a difference of dispensable and indispensable monomials, or (iii) a difference of two indispensable monomials. The situations where each case arises are shown in Proposition 4.3 and in Proposition 4.1. We have found some examples for the case (ii) by introducing some structural zero cells for the case (i),

The enumeration of indispensable monomials seems a very important problem, since it can lead directly to the enumeration of indispensable binomials. In addition, it also gives the fibers of the special structure that it contains at least one singleton equivalence class. Moreover, by finding dispensable binomials which are differences of two indispensable monomials, we can find all fibers that only contain singleton equivalence classes.

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